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This article introduces a stochastic thermodynamics for driven out-of-equilibrium open quantum systems. A stochastic Schrödinger equation allows to construct quantum trajectories describing the dynamics of the system state vector in presence of an environment. Thermodynamic quantities are then defined at the single quantum trajectory level. We thereby identify coherent contributions, without classical counterparts, leading to quantum fluctuations of thermodynamic quantities. This formalism eventually leads to central fluctuation theorems for entropy, extending in the quantum regime results obtained in classical stochastic thermodynamics. The thermal imprint of coherences on a simple implementation of Jarzynski equality is investigated, opening avenues for a thermodynamic approach to decoherence.

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Thermodynamics arose in the 19th century as a powerful theory to describe energy exchanges in thermal engines [1]. While its domain of application has grown to encompass for instance transfer and conversion of information [2], extension to out-of-equilibrium systems remains a challenge. To this end, stochastic thermodynamics has emerged as a compelling thermodynamics approach to small, out-of-equilibrium classical systems by giving a central role to trajectories [3–5]. The basic idea is to associate thermodynamic quantities to stochastic trajectories in the system phase space. Equilibrium then simply appears as the particular case of trajectories reduced to a single point. Both the trajectory and its probability are used to define thermodynamic quantities such as heat, work and entropy at the single trajectory level, allowing for the enunciation of the first principle of thermodynamics [3]. Time reversal operation then leads to central fluctuation theorems: The second law of thermodynamics and other celebrated fluctuation theorems such as Jarzynski [6] and Crooks [7] relations then appear as particular cases of these central fluctuation theorems [4], highlighting the unifying strength of stochastic thermodynamics. Meanwhile experimental realizations of quantum devices [8] have called for a thermodynamic description of quantum systems [9], to address questions such as efficiency of quantum machines [10, 11]. While significant theoretical contributions have been made using a broad range of definitions and concepts [12–14], a unified and consistent theoretical framework describing energy, entropy and their fluctuations at the single trajectory level, is still lacking. Here we set the foundations of a stochastic thermodynamics for driven out-of-equilibrium open quantum systems, based on quantum trajectories. Introduced first in quantum optics [15, 16], they have become a standard tool to monitor and control quantum systems [17–20] and are used here to define thermodynamic quantities at the single trajectory level. After defining the system and its environment, we introduce the stochastic Schrödinger equation, playing the role of the Langevin equation in the classical case to generate stochastic trajectories of the system. We then define its internal energy whose variations along a single trajectory lead to definitions for generalized work and heat and an expression of the 1^{st} principle of thermodynamics at the single trajectory level. We eventually focus on the particular case of an environment at thermal equilibrium and use a notion of time reversal to derive central fluctuation theorems and the second law of thermodynamics. A simple implementation of Jarzynski equality in the presence of quantum coherences is proposed, a first step towards observing energetic clues of decoherence.

System and model – The generic system under study is a n_{s}-level quantum system, described by a state vector belonging to a Hilbert space $\mathcal{H}$. Our system is open in two different ways. Firstly, it can be driven by an external operator through a time-dependent Hamiltonian $\hat{H}_{\text{s}}(t)$. Secondly, the system is also in contact with a reservoir, involving an infinite number of degrees of freedom and modeled as a Markovian bath with strictly zero memory time. This reservoir is not necessarily at thermal equilibrium, and can eventually be monitored, *i.e.* continuously measured in various eigenbasis. The system density matrix $\rho_{\text{s}}(t)$ is obtained by tracing out the reservoir degrees of freedom. Lindblad proved that the most general Markovian master equation for $\rho_{\text{s}}(t)$ reads [21]

$$\partial_t \rho_{\text{s}}(t) = -\frac{i}{\hbar}[\hat{H}_{\text{s}}(t), \rho_{\text{s}}(t)] + \sum_{\mu=1}^{n} \left(\hat{L}_\mu(t) \rho_{\text{s}}(t) \hat{L}_\mu^\dagger(t) \right) - \frac{1}{2} \sum_{\mu=1}^{n} \left(\hat{L}_\mu^\dagger(t) \hat{L}_\mu(t) \rho_{\text{s}}(t) + \rho_{\text{s}}(t) \hat{L}_\mu^\dagger(t) \hat{L}_\mu(t) \right), \quad (1)$$

introducing a set of at most $n = n_{\text{s}}^2 - 1$ jump operators $\hat{L}_\mu(t)$ acting on $\mathcal{H}_{\text{s}}$. In general the jump operators are

explicitly time-dependent [22], but from now on we will not write this time-dependence explicitly to simplify notations.

In order to build a framework analogous to classical stochastic thermodynamics, it is convenient to work with a quantum analogue of the Langevin equation, describing the dynamics of the system state vector itself rather than its density matrix. This is achieved by unraveling the Lindblad equation [23–25] to generate stochastic trajectories of the state vector in the system Hilbert space, $\gamma : t \in [t_\mathrm{i} : t_\mathrm{f}] \to |\psi\,(t,\vec{\mu})\rangle$, under the influence of an ordered sequence $\vec{\mu}$ of jump operators. The system dynamics must be consistent with the Lindblad equation after averaging on all possible interaction sequences $\vec{\mu}$. In the continuous-time limit such dynamics leads to the so-called Linear Stochastic Schrödinger Equation (LSSE) for the system state vector [23]:

$$d|\psi\,(t,\vec{\mu})\rangle = -\frac{idt}{\hbar}\hat{H}_\mathrm{eff}(t)|\psi\,(t,\vec{\mu})\rangle + d\hat{D}(t)|\psi\,(t,\vec{\mu})\rangle. \quad (2)$$

The first term in this equation corresponds to a deterministic dynamics governed by a non-Hermitian effective Hamiltonian $\hat{H}_\mathrm{eff}(t) = \hat{H}_\mathrm{s}(t) + i\hbar\hat{J}$, with $\hat{J} = -\frac{1}{2}\sum_{\mu=1}^{n} L_\mu^\dagger L_\mu$. The second term describes the random action of the reservoir on the system, represented by the stochastic operator $d\hat{D}(t) = \sum_{\mu=1}^{n} dN_\mu(t)\hat{E}_\mu(t)$. Each operator $\hat{E}_\mu(t)$ can be seen as the back action on the system dynamics of transitions in the environment and is related to a jump operator $\hat{L}_\mu$, its precise expression depending on the interaction between the system and the reservoir [25]. We briefly present here the two main classes of quantum trajectories considered. Quantum jumps unraveling corresponds to a reservoir performing projective measurements on the system. Then $dN_\mu(t) \in \{0,1\}$ are Poisson processes with $\mathbb{E}\left[dN_\mu(t)\right] = \gamma_\mu dt$, and $\hat{E}_\mu = \frac{\hat{L}_\mu}{\sqrt{\gamma_\mu}} - \mathbb{1}_\mathrm{s}$. Quantum state diffusion corresponds to a reservoir performing weak measurements on the system. Then $dN_\mu(t)$ are complex Gaussian processes, defined by $\mathbb{E}\big[dN_\mu(t)\big] = 0$, $\mathbb{E}\big[dN_\mu(t)dN_\nu(t')\big] = 0$ and $\mathbb{E}\big[dN_\mu(t)dN_\nu^*(t')\big] = \delta_{\mu\nu}\delta(t-t')dt$, and $\hat{E}_\mu = \hat{L}_\mu$. For a given realization, the system remains in a pure state all along its trajectory, but each realization leads to a different pure state trajectory. Note that the theoretical framework presented here does *not* rely on the particular choice of unraveling but only on the existence of stochastic differential equation (Eq.2) in the Hilbert space. Figure 1(a) presents an example of a quantum trajectory for a Qubit undergoing quantum state diffusion induced by the reservoir [25].

The evolution described by Eq.2 can be seen as the continuous time limit of a discrete process: If one discretizes the time interval between $t = t_\mathrm{i}$ and $t = t_\mathrm{f}$ into N time intervals, at each time t_k, the jump operator applied at time t_k is $\hat{L}_{\mu(t_k)}$ if the reservoir induces a jump $\mu(t_k) \neq 0$ on the system, while if no jump occurs at this time one applies the no-jump operator $\hat{L}_0 = \mathbb{1} - \frac{idt}{\hbar}\hat{H}_\mathrm{s}(t_k) - \frac{dt}{2}\sum_{\mu=1}^{n} L_\mu^\dagger L_\mu$. The state vector then evolves under the joint influence of the time-dependent Hamiltonian and a time-ordered sequence $\vec{\mu}$ of N operators, leading to the final state vector

$$|\psi\,(t_\mathrm{f},\vec{\mu})\rangle = \hat{L}_{\mu(t_N)}\cdots\hat{L}_{\mu(t_1)}|\psi_\mathrm{i}\rangle = \prod_{k=1}^{\overleftarrow{N}}\hat{L}_{\mu(t_k)}|\psi_\mathrm{i}\rangle. \quad (3)$$

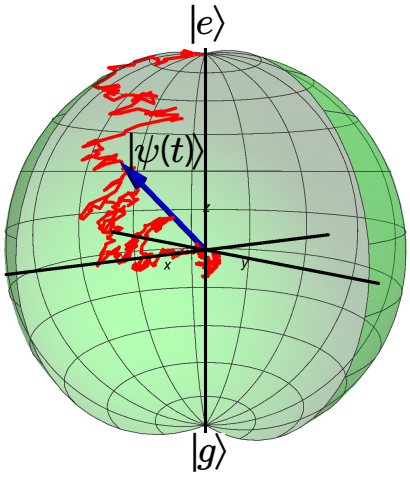
Note that with this particular choice of description, the state vector right after the application of a jump operator is not normalized [23]. As a result its norm is not conserved during this process: actually the squared norm of state vector $|\psi\,(t,\vec{\mu})\rangle$ at time t is nothing but the joint probability of the jump operators sequence bringing the initial state vector $|\psi_\mathrm{i}\rangle$ to $|\psi\,(t_\mathrm{f},\vec{\mu})\rangle$. Consequently, the probability of a trajectory γ is $P[\gamma] \overset{\mathrm{def}}{=} \langle\psi\,(t_\mathrm{f},\vec{\mu})\,|\psi\,(t_\mathrm{f},\vec{\mu})\rangle$ and can be used to define the *entropy of a trajectory* by analogy with classical stochastic thermodynamics [4], as the negative log-likelihood or surprisal [26] of the trajectory $S(t) = -\ln P[\gamma]$. We shall later see that this entropy does not identify with the system thermodynamic entropy, just like in the classical case [4].

In the following we shall consider the situation where a system described by a state vector $|\psi_\mathrm{i}\rangle$ at time $t = t_\mathrm{i}$ evolves under the joint action of a reservoir and an operator aiming at reaching a target state $|\psi_\mathrm{t}\rangle$ at time $t = t_\mathrm{f}$. Again the norm of these states gives their probabilities, $P_{\mathrm{i/t}} = \langle\psi_{\mathrm{i/t}}|\psi_{\mathrm{i/t}}\rangle$, equal for instance to 1 if the system is prepared in a pure state, or to a Gibbs weight for a thermal mixture. The stochastic Schrödinger equation then generates a bundle of quantum trajectories starting in $|\psi_\mathrm{i}\rangle$, corresponding to different realizations of the stochastic operator $d\hat{D}(t)$. We shall now see it makes a trajectory approach to quantum open systems particularly suitable to define thermodynamic quantities that are not state functions, such as heat or work [27].

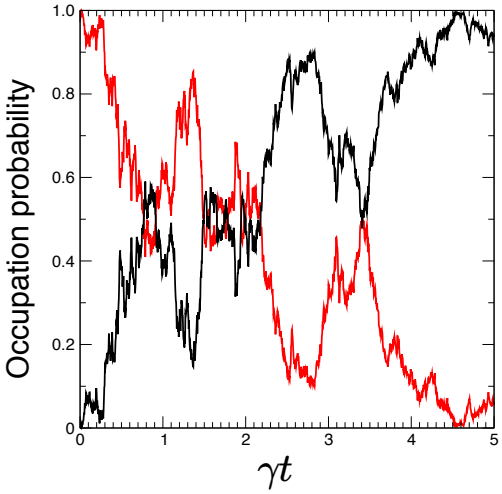
Thermodynamics of quantum trajectories – We now characterize exchanges of energy at the single quantum trajectory level, in analogy with classical stochastic energetics [3]. We propose to use as a thermodynamic potential the expected value of the system energy in state $|\psi\,(t,\vec{\mu})\rangle$, defined as

$$U(t) \overset{\mathrm{def}}{=} \langle\hat{H}_\mathrm{s}(t)\rangle_{\psi_t} = \frac{\langle\psi\,(t,\vec{\mu})\,|\hat{H}_\mathrm{s}(t)|\psi\,(t,\vec{\mu})\rangle}{\langle\psi\,(t,\vec{\mu})\,|\psi\,(t,\vec{\mu})\rangle}. \quad (4)$$

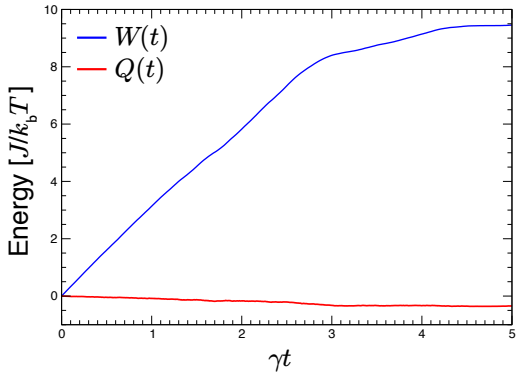
Note that this quantity, hereafter called internal energy, can not be obtained as result of a single energy measurement of the system, unless the system is in a eigenstate of Hamiltonian $\hat{H}_\mathrm{s}(t)$. However, it can be fully inferred from the knowledge of the applied time-dependent Hamiltonian $\hat{H}_\mathrm{s}(t)$ and the quantum trajectory of the system at each time of the transformation. Generalized work and



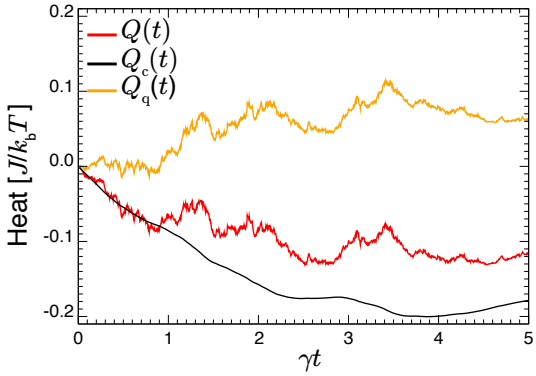
(a) Quantum trajectory in the Bloch sphere



(b) Populations dynamics



(c) Integrated work and heat



(d) Classical and quantum contributions to heat

FIG. 1: **Application to a Qubit**. A two-level system with Hamiltonian $\hat{H}_s(t) = \Delta(t)|e\rangle\langle e|$, with a set of only two jump operators, $\hat{L}_1 = \sqrt{\gamma_1}|e\rangle\langle g|$ and $\hat{L}_2 = \sqrt{\gamma_2}|g\rangle\langle e|$, corresponding respectively to transition from the ground state to the excited state, and to the opposite transition. The gap varies with time as $\beta\Delta(t) = \beta\Delta_0(1 + \alpha\gamma t)$, with $\gamma = \gamma_2 - \gamma_1$, by applying an external field (here $\beta\Delta_0 = 10^{-1}$ and $\alpha = 7.3 \times 10^{-1}$). **a**: Example of quantum trajectory, representing the quantum state diffusion [25] of the state vector in the Bloch sphere as a function of time. The system is initially in the pure state $|e\rangle$, and evolves according to LSSE (Eq.2) along the quantum trajectory represented by the red line. The blue arrow represents the system state vector at some intermediate time. Note that in contrast with the case of an isolated Qubit, the trajectory does not remain at the Bloch sphere surface but gets *inside* the sphere, a signature of decreasing purity. **b**: Dynamics of the occupation probabilities of the ground state $p_g(t) = \langle|g\rangle\langle g|\rangle_{\psi_t}$ (black) and the excited state $p_e(t) = \langle|e\rangle\langle e|\rangle_{\psi_t}$ (red) as a function of time, showing the Qubit relaxation from its excited state to the ground state. **c**: Time-evolution of the work $W(\gamma t) = \int_0^{\gamma t} \delta W(u)$, where $\delta W(u) = \langle\delta\hat{W}(u)\rangle_{\psi_u} = p_e(u)\dot{\Delta}(u)du$ here, and the heat $Q(\gamma t) = \int_0^{\gamma t} \delta Q(u)du$ along the trajectory represented in Fig.1(a). **d**: Decomposition of heat in classical and quantum contributions. Elementary heat, $\delta Q(u) = \langle\delta\hat{Q}\rangle_{\psi_u}$, can be decomposed in two contributions, $\delta Q = \delta Q_c + \delta Q_q$, where $\delta Q_c = \Delta(t)dt\,[\gamma_1 p_g(t) - \gamma_2 p_e(t)]$ is a classical contribution involving only populations (black line) whereas $\delta Q_q = \Delta(t)\left[p_{eg}(t)\left(p_g d\omega_1\sqrt{\gamma_1} - p_e d\omega_2^*\sqrt{\gamma_2}\right) + \text{c.c.} - 2p_{eg}(t)p_{ge}(t)dt(\gamma_1 p_g(t) - \gamma_2 p_e(t))\right]$ is a purely quantum contribution coming from the coherences, $p_{eg}(t) = \langle|e\rangle\langle g|\rangle_{\psi_t}$ (orange). Time-evolution of the total heat $Q(\gamma t)$ along the same trajectory is represented in red.

heat are then defined as the two ways by which internal energy can change during a time interval dt, and their expressions identified by differentiation of $U(t)$, using Itō's convention for stochastic terms [28].

The elementary generalized work, performed by an external operator applying a given protocol to drive the system, is here defined as the contribution to the differential associated with the Hamiltonian variation during dt. It can be written as the expectation of an elementary operator, $\delta W(t) = \langle \delta\hat{W}(t)\rangle_{\psi_t}$, where we introduced the elementary work operator $\delta\hat{W}(t) = d\hat{H}_{\rm s}(t)$. This work operator can be decomposed on the instantaneous basis of the Hamiltonian eigenstates, and includes in general coherent contributions with no classical equivalents.

The elementary generalized heat is defined as the sum of all remaining contributions, and includes in particular the exchange of energy with the reservoir. It can also be written as $\delta Q(t) = \langle \delta\hat{Q}(t)\rangle_{\psi_t}$, where $\delta\hat{Q}(t)$ is the elementary generalized heat operator. Introducing $\hat{\Delta}_{\rm s}(t) = \hat{H}_{\rm s}(t) - U(t)\mathbb{1}_{\rm s}$, $d\mu(t) = \langle d\hat{D}(t) + d\hat{D}^\dagger(t)\rangle_{\psi_t}$, and notation $[\cdots]_1$ to mention that the term between brackets must be expanded up to stochastic terms of order dt, we have:

$$\delta\hat{Q}(t) = \hat{\Delta}_{\rm s}(t)\left(d\hat{D}(t) + \hat{J}dt\right) + {\rm hc} + \left[d\hat{D}^\dagger(t)\hat{\Delta}_{\rm s}(t)d\hat{D}(t)\right]_1 - d\mu(t)\left[\left(\hat{\Delta}_{\rm s}(t)d\hat{D}(t) + d\hat{D}^\dagger(t)\hat{\Delta}_{\rm s}(t)\right)\right]_1 . \quad (5)$$

One can decompose the generalized elementary heat into a classical part $\delta Q_{\rm c}(t)$, depending on system populations, and a genuinely quantum contribution $\delta Q_{\rm q}(t)$ involving quantum coherences. If the system is in a superposition of energy eigenstates, $Q_{\rm q}$ is non-zero at the single trajectory level and leads to quantum heat fluctuations. The conservation of internal energy finally reads $dU(t) = \delta W(t) + \delta Q(t)$. Generalized work along a quantum trajectory γ is $W[\gamma] = \int_{t_{\rm i}}^{t_{\rm f}} \langle \delta\hat{W}(t)\rangle_{\psi_t}$ while generalized heat is $Q[\gamma] = \int_{t_{\rm i}}^{t_{\rm f}} \langle \delta\hat{Q}(t)\rangle_{\psi_t}$. Note that these quantities are not state functions since they depend on the whole trajectory γ and not only on its starting and ending points [27]. We then obtain the following expression for the 1$^{\rm st}$ principle of thermodynamics at the single trajectory level:

$$\Delta U = W[\gamma] + Q[\gamma]. \quad (6)$$

An implementation of this framework with a Qubit is presented in Fig.2 to study a simple Landauer erasing protocol. It provides an energetic point of view to quantum operations and opens avenues for further investigations of quantum thermal machines.

We stress here that alternative and equally valid definitions for heat and work can be used to build a consistent theory. Depending on chosen definitions, work can exhibit different properties and may satisfy fluctuation relations or not as discussed for example in [29]. In particular, our definition of work is different from other approaches based on the two-points measurement protocol [27, 30], relying on projective measurements of the system or reservoir energy at the beginning and the end of the transformation. In the spirit of stochastic thermodynamics [3, 4], our formalism is based on the ability to monitor the stochastic dynamics of the system observables: this approach is therefore particularly suitable for experiments giving access to the system quantum trajectories [17–20].

A simple example – One can get a first glimpse on this formalism ability to describe purely quantum effects by considering the canonic example of the spontaneous emission of a Qubit [31], initially prepared in a coherent superposition $|\psi_{\rm i}\rangle = (|e\rangle + |g\rangle)/\sqrt{2}$, where $|g\rangle$ and $|e\rangle$ are respectively the Qubit ground state and excited state. Here no work is performed on the system ($W = 0$), and the bath at zero temperature is monitored in its energy eigenbasis using a photon counter, corresponding to a quantum jumps unraveling [32]. The Qubit relaxes to its ground state when time goes to infinity, so that $\Delta U = -\hbar\omega_0/2$ for each trajectory. Let us now consider the subset of trajectories where no photon were emitted. One can show that for such "no-jump" trajectories, the heat has no classical component $Q_{\rm c}[\gamma] = 0$. Nevertheless the state vector evolves, not because of spontaneous emission events but rather because knowledge about the system changes: the longer one waits without detecting photon emission, the more likely it gets that the system is actually in its ground state. The exchanged heat is non-zero due to this continuous state evolution and reads: $Q[\gamma] = Q_{\rm q}[\gamma] = \Delta U = -\hbar\omega_0/2$.

To understand the origin of this quantum heat $Q_{\rm q}[\gamma]$, it is actually necessary to take into account the energy provided by the source used to prepare the coherent superposition at time $t < 0$. At $t = 0^-$, the source and the system are weakly entangled: Their global state is a coherent superposition where the source has equal chance to provide no energy (if the qubit is in $|g\rangle$) or an energy $\hbar\omega_0$ (if the qubit is in $|e\rangle$). At this time an energy $\hbar\omega_0$ is equally shared between the system and the source, which corresponds to an average work performed by the source $\hbar\omega_0/2$. Note that weak entanglement is fully compatible with a Qubit being in a pure state, as long as the source initial state is quasi classical (see Supplementary Material for an analysis in Cavity QED). Not detecting the Qubit in state $|e\rangle$ amounts to project the superposition on the Qubit ground state $|g\rangle$, in which case where the source provides no energy. The quantum heat is the necessary energy contribution due to the projection induced by the measurement.

As it appears from the previous example, quantum heat appears if the reservoir naturally induces transitions in a basis where the system state has coherences, and can ultimately be seen as the signature of a mismatch between

the basis in which the system is prepared, and the basis in which the reservoir measures. For instance, in the simple case described above, the Qubit is prepared in the σ_x basis, while the reservoir induces transitions in the σ_z basis. In the same way, quantum heat can also appear when the system state is prepared in an eigenstate of the Hamiltonian, and the reservoir induces transitions in a different basis than the energy basis, as in the case for quantum state diffusion (See Fig.2d).

Fluctuation theorems – We now turn to entropy consideration and fluctuation theorems. Thermodynamic entropy is tightly related to irreversibility: A physical process is said reversible if the surprisal takes the same value $S(t)$ for the forward and backward trajectories. This remark highlights that the surprisal of a quantum trajectory has to be supplemented with a notion of time reversal to acquire a proper thermodynamic interpretation. From now on we shall make further assumptions about the reservoir and consider only a thermal bath, weakly coupled to the system and at equilibrium, therefore represented by a stationary Gibbs state at temperature T. Note that these additional assumptions are more restrictive than the simple Markov assumption used to express the 1$^{\text{st}}$ principle at the trajectory level.
We then adopt a notion of time reversal [33] already used to derive fluctuation relations for open quantum systems [29]. During the forward process the system follows the forward trajectory γ, which can be represented by an initial state $|\psi_{\rm i}\rangle$, a sequence $\vec{\mu}$ of jump operators $\hat{L}_\mu$ and a target state $|\psi_{\rm t}\rangle$: $\gamma \equiv \{\psi_{\rm i}, \vec{\mu}, \psi_{\rm t}\}$. The corresponding reversed trajectory, $\gamma_{\rm r} \equiv \{\psi_{\rm t}, \vec{\mu}_{\rm r} = \overleftarrow{\mu}, \psi_{\rm i}\}$, is generated by the reversed sequence of time-reversed jump operators $\hat{L}^{\rm r}_\mu$ given by $\hat{L}^{\rm r}_\mu = \hat{L}^\dagger_\mu \exp\left(\frac{\beta}{2}\delta E_{{\rm res},\mu}\right)$ [29, 33]. Here the reservoir undergoes a transition from its eigenstate $|b_i\rangle$(energy $E_i^{\rm res}$) to $|b_j\rangle$ (energy $E_j^{\rm res}$), and acts on the system with $\hat{L}_\mu = \hat{L}_{ij}$. The term $\delta E_{{\rm res},\mu} = E_i^{\rm b} - E_j^{\rm b}$ is the energy change of the reservoir induced by the transition, and is part of the elementary heat received by the reservoir (in the direct process). The probability of trajectory γ during the forward process is given by

$$P_{\rm d}[\gamma] \stackrel{\rm def}{=} P_{\rm i}(\psi_{\rm i})\langle\psi_{\rm t}|\prod_{k=1}^{\overleftarrow{N}}\hat{L}_{\mu_k}(t_k)|\psi_{\rm i}\rangle\langle\psi_{\rm i}|\prod_{k=1}^{\overrightarrow{N}}\hat{L}^\dagger_{\mu_k}(t_k)|\psi_{\rm t}\rangle,$$

while the probability of $\gamma_{\rm r}$ reads

$$\begin{aligned} P_{\rm r}[\gamma_{\rm r}] &\stackrel{\rm def}{=} P_{\rm t}(\psi_{\rm t})\langle\psi_{\rm i}|\prod_{k=1}^{\overleftarrow{N}}\hat{L}^{\rm r}_{\mu_k}(t^{\rm r}_k)|\psi_{\rm t}\rangle\langle\psi_{\rm t}|\prod_{k=1}^{\overrightarrow{N}}\hat{L}^{\dagger{\rm r}}_{\mu_k}(t^{\rm r}_k)|\psi_{\rm i}\rangle, \\ &= \frac{P_{\rm t}(\psi_{\rm t})}{P_{\rm i}(\psi_{\rm i})}\exp\left[-\beta\Delta E_{\rm res}[\gamma]\right]P_{\rm d}[\gamma], \end{aligned}$$

where $\Delta E_{\rm res}[\gamma] = \sum_{k=1}^N \delta E_{{\rm res},\mu}$ is the total energy variation of the reservoir. We can then define the corresponding entropy variation in the reservoir at temperature T, $\Delta S_{\rm res}[\gamma] = \Delta E_{\rm res}[\gamma]/T$. We can also define the change in system entropy by $\Delta S_{\rm sys}[\gamma] \stackrel{\rm def}{=} -k_{\rm b}\ln\left(\frac{P_{\rm t}(\psi_{\rm t})}{P_{\rm i}(\psi_{\rm i})}\right)$. Defining then the total entropy variation along the trajectory as $\Delta S_{\rm tot}[\gamma] \stackrel{\rm def}{=} \Delta S_{\rm sys}[\gamma] + \Delta S_{\rm res}[\gamma]$ leads to the detailed central fluctuation theorem

$$P_{\rm r}[\gamma_{\rm r}] = \exp\left[-\Delta S_{\rm tot}[\gamma]/k_{\rm b}\right]P_{\rm d}[\gamma]. \tag{7}$$

Averaging over all possible trajectories γ leads to the integral central fluctuation theorem

$$\left\langle e^{-\Delta S_{\rm tot}[\gamma]/k_{\rm b}}\right\rangle = 1. \tag{8}$$

In particular the second law of thermodynamics follows from convexity of the exponential:

$$\langle\Delta S_{\rm tot}[\gamma]\rangle \geq 0. \tag{9}$$

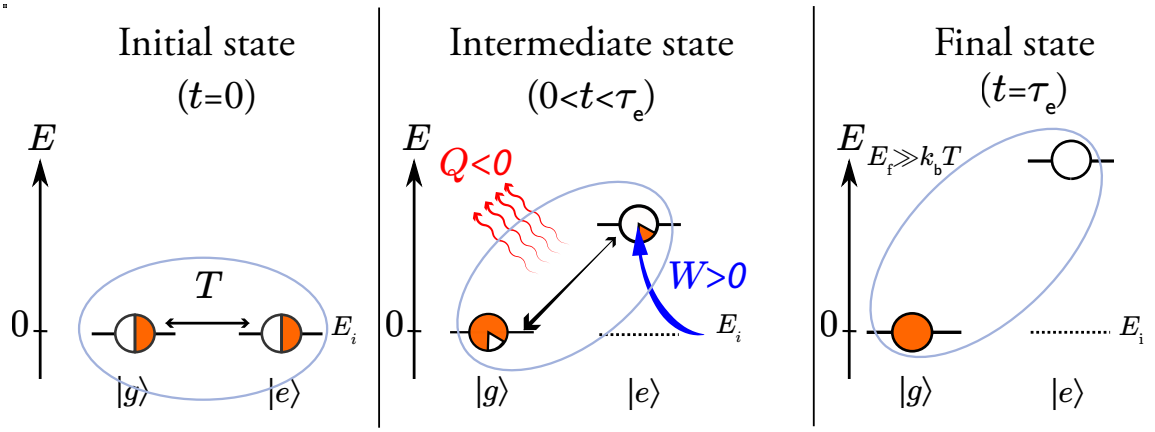
We term the two relations Eq.7 and Eq.8 *central fluctuation theorems* as other fluctuation relations derive from these main relations.

Jarzynski relation – For the sake of clarity, we shall assume from now on that the reservoir undergoes strong measurements it its energy eigenbasis, which corresponds to the recording of counting statistics [30]. On the system side, such monitoring corresponds to a quantum jump unraveling. This monitoring scheme is perfectly compatible with thermal equilibrium, and it allows in particular direct access to the energy change in the reservoir $\Delta E_{\rm res}[\gamma]$, which is of critical importance for experimental verification of Jarzynski equality. As usual for this equality, we assume that initial states for both the forward trajectory, $|\psi_{\rm i}\rangle$, and the backward trajectory, $|\psi_{\rm t}\rangle$, are eigenstates of the initial and final system Hamiltonians, drawn from equilibrium distributions at the same temperature T, then $P_{\rm i/t}(\psi_{\rm i/t}) = Z_{\rm i/t}(T)^{-1}\exp\left(-\beta\epsilon_{\rm i/t}\right)$, where $\hat{H}_{\rm s}(t_{\rm i}/t_{\rm t})|\psi_{\rm i/t}\rangle = \epsilon_{\rm i/t}|\psi_{\rm i/t}\rangle$ and $\beta = 1/k_{\rm b}T$. The 1$^{\text{st}}$ law of thermodynamics at the single trajectory level reads $\Delta U = \epsilon_{\rm t} - \epsilon_{\rm i} = W[\gamma] + Q[\gamma]$. Introducing the system free energy F defined as $\beta F \stackrel{\rm def}{=} -\ln Z$, the integral central fluctuation theorem eventually leads to a generalized Jarzynski identity

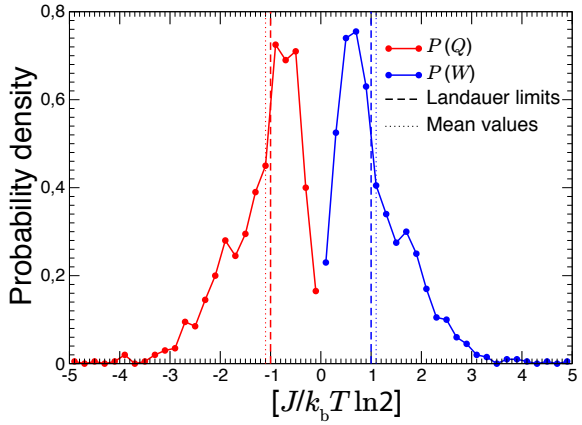
$$\langle\exp\left(-\beta W_{\rm eff}[\gamma]\right)\rangle = \exp\left(-\beta\Delta F\right), \tag{10}$$

where the effective work $W_{\rm eff}[\gamma]$ is defined as $W_{\rm eff}[\gamma] = W[\gamma] + Q[\gamma] - \Delta E_{\rm res}[\gamma]$.

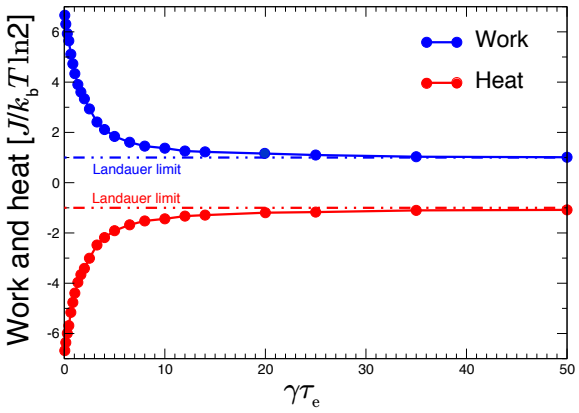
The classical Jarzynski relation [6] is recovered in the particular case where $Q[\gamma] = \Delta E_{\rm res}[\gamma]$. Both in classical and quantum regimes, such an equality requires the additivity of the system and reservoir energies, which is the case in the weak coupling regime under study. More importantly, and specifically to the quantum case, it also requires that global energy of the system and the reservoir is conserved when a quantum jump takes place,



(a) Schematic presentation of the protocol



(b) Probability distribution of total heat $Q(\tau_e)$ and work $W(\tau_e)$



(c) Evolution of averaged work and heat

FIG. 2: **Landauer erasing protocol**. **a**: Schematic presentation of the protocol. Starting with a mixed state of $|e\rangle$ and $|g\rangle$, the operator rises the excited state energy between $t = 0$ and $t = \tau_e$, starting from $E_i = k_b T/10$ to $E_f = 10 k_b T$, thus providing work to the system ($W > 0$). The thermostat then allows the system to make transitions from $|e\rangle$ to $|g\rangle$ (state occupation is represented by the disk colored portion), creating a heat flow from the system to the bath ($Q < 0$). In the final state, the excited state energy is $E_f \gg k_B T$ and the system is in its ground state, regardless of its initial state. **b**: Probability distribution of total heat $Q(\tau_e)$ and work $W(\tau_e)$, for $\gamma\tau_e = 25$. Vertical dotted lines represent the expected values $\mathbb{E}[Q(\tau_e)]$ and $\mathbb{E}[W(\tau_e)]$ from an ensemble of trajectories. The vertical dashed lines represent Landauer limits for a quasi-static process ($\tau_e \to \infty$). **c**: Evolution of $\mathbb{E}[Q(\tau_e)]$ and $\mathbb{E}[W(\tau_e)]$, showing the convergence towards Landauer limits for a quasi-static process, $\mathbb{E}[W(\tau_e \to \infty)] = -\mathbb{E}[Q(\tau_e \to \infty)] = k_b T \ln 2$.

which requires in particular that the system state has no coherences in the energy eigenbasis: A counter-example if the system has such coherences is analyzed below. The classical regime is realized in most recent experimental investigations of the extensions of Jarzynski equality for quantum systems [34–36].

Quantum coherences and Jarzynski equality – To highlight the deviations induced by quantum coherences, we shall consider again the example of a Qubit, now coupled to a heat bath of temperature T. At $t = 0$ the Qubit is at equilibrium with the bath. From $t = 0^+$ to $t = T_{\pi/2}$, the Qubit is coupled to a resonant classical source performing the coherent transformation $|g\rangle \to |+_x\rangle = (|e\rangle + |g\rangle)/\sqrt{2}$, and $|e\rangle \to |-_x\rangle = (-|e\rangle + |g\rangle)/\sqrt{2}$. The necessary time to perform the $\pi/2$ pulse is supposed very short with respect to the typical time of the relaxation induced by the bath, such that relaxation can be safely be neglected. At $t = T_{\pi/2}$ the source is decoupled and the system remains solely in contact with the heat bath, so that the Qubit slowly gets back to equilibrium. As the system Hamiltonian is the same at the initial and final times of this transformation, one gets $\Delta F = 0$. Work is only performed while the source is coupled, and equals $W_g = \hbar\omega_0/2$ if the qubit is initially in $|g\rangle$ with probabil-

$\|\psi_i\rangle$	1st jump	Q	W	$\Delta E_{\rm res}$	$W_{\rm eff}$	Probability
$\|g\rangle$	$\uparrow$	$\frac{\hbar\omega_0}{2}$	$\frac{\hbar\omega_0}{2}$	$\hbar\omega_0$	0	$\frac{1}{2}\frac{e^{-\hbar\beta\omega_0}}{1+e^{-\hbar\beta\omega_0}}$
$\|g\rangle$	$\downarrow$	$-\frac{\hbar\omega_0}{2}$	$\frac{\hbar\omega_0}{2}$	$-\hbar\omega_0$	$\hbar\omega_0$	$\frac{1}{2}\frac{e^{-\hbar\beta\omega_0}}{1+e^{-\hbar\beta\omega_0}}$
$\|e\rangle$	$\uparrow$	$\frac{\hbar\omega_0}{2}$	$-\frac{\hbar\omega_0}{2}$	$\hbar\omega_0$	$-\hbar\omega_0$	$\frac{1}{2}\frac{1}{1+e^{-\hbar\beta\omega_0}}$
$\|e\rangle$	$\downarrow$	$-\frac{\hbar\omega_0}{2}$	$-\frac{\hbar\omega_0}{2}$	$-\hbar\omega_0$	0	$\frac{1}{2}\frac{1}{1+e^{-\hbar\beta\omega_0}}$

TABLE I: Heat, work, change of reservoir energy, effective work and weight in the Jarzinsky equality for the example of the qubit driven by a classical coherent source.

ity $p_g^{\rm eq} = 1/(1+e^{-\beta\hbar\omega_0})$, and $W_e = -\hbar\omega_0/2$ if the qubit is initially in state $|e\rangle$ with probability $p_e^{\rm eq} = 1 - p_g^{\rm eq}$. In this situation it is clear that $\langle e^{-\beta W[\gamma]}\rangle \neq 1$, calling for quantum corrections.

Following the previous analysis, we now consider the effective work $W_{\rm eff}[\gamma] = W[\gamma] + Q[\gamma] - \Delta E_{\rm res}[\gamma]$. Let us first consider the case where the Qubit is initially in $|g\rangle$, which happens with probability $p_g^{\rm eq}$. The source provides a work $W_g = \hbar\omega_0/2$ to prepare the Qubit in the state $|+_x\rangle$. When the first jump takes place, the Qubit can be projected on $|e\rangle$ while absorbing a photon of the bath. At this step the trajectory has a probability $p_g^{\rm eq}/2$ (see Appendix for a detailed calculation of the trajectory probabilities). After the first jump, the heat reads $Q = \hbar\omega_0/2$, while $\Delta E_{\rm res} = \hbar\omega_0$. The difference $Q - \Delta E_{\rm res} = -\hbar\omega_0/2$ is nothing but the quantum component of the elementary heat. The heat exchanges in the rest of the trajectory satisfy $Q'[\gamma] = \Delta E'_{\rm res}[\gamma]$: There is no quantum contribution anymore as the Qubit is always in one of its energy states. The effective work eventually reads $W_{\rm eff} = 0$: It quantifies the work effectively performed by the source after the measurement projection. The three other cases respectively correspond to a Qubit initially in $|g\rangle$ and projected in $|g\rangle$, and a Qubit initially in $|e\rangle$, projected in $|e\rangle$ or $|g\rangle$. Values for heat, work and effective work, as well as the probability of each trajectory are detailed in the table I. One easily checks that $\langle e^{-\beta W_{\rm eff}[\gamma]}\rangle = 1$, showing the importance of quantum corrections to fluctuation theorems.

As in the case of classical systems [4, 6, 7], the derivation of fluctuation relations clearly highlights that they merely express the constraints imposed on the system dynamics by an environment *at equilibrium*. If one aims at probing these fluctuation relations within a given experimental set-up, the measurement channel must be taken into account in the environment of the system. If counting statistics are compatible with thermal equilibrium as stated above, in general other monitoring schemes are expected to perturb this equilibrium and the above fluctuation relations have no reason to hold anymore. This difference is another clear consequence of the disruptive nature of measurements in quantum mechanics: Taking them into account is a major challenge for future researches in quantum thermodynamics.

In this article we propose a consistent theoretical framework for a trajectory-based out-of-equilibrium thermodynamics for driven open quantum systems. It allows one to define thermodynamic quantities at the single trajectory level and to quantify their fluctuations, therefore transposing in the quantum regime the theoretical appeal of classical stochastic thermodynamics. However the strength of the latter theory comes from its experimental implementation to analyze out-of-equilibrium systems [5], using particle tracking techniques to record trajectories and estimate thermodynamic quantities. In the quantum regime, an experimental implementation requires the reconstruction of an ensemble of quantum trajectories [19] and estimate thermodynamic quantities from these trajectories. If such a program remains an experimental challenge, recent progress in monitoring quantum systems puts this goal within reach [19, 20]. Quantum stochastic thermodynamics associated with these techniques holds the promise to provide a comprehensive description of out of equilibrium quantum systems, and a thermodynamic perspective on quantum computing, quantum measurement and decoherence.

Appendix – We compute here the probability of the different values the effective work $W_{\rm eff}$ can take in the example of the last section. We consider a Qubit initially in equilibrium with a thermal bath at temperature T and focus on a trajectory starting in the ground state, such that the initial Qubit state $|\psi_{\rm i}\rangle$ is $\sqrt{p_g^{\rm eq}}|g\rangle$, with $p_g^{\rm eq} = (1+e^{-\beta\hbar\omega_0})^{-1}$ the probability for that initial state to be drawn from the thermal mixture. The Qubit then interacts with a classical source for a time $T_{\pi/2}$. The result is state $\sqrt{p_g^{\rm eq}}|+_x\rangle$, where $|+_x\rangle = (|e\rangle + |g\rangle)/\sqrt{2}$. The Qubit then remains in contact with the thermal bath, so that it evolves according to the effective hamiltonian $\hat{H}_{\rm eff} = (\omega_0 - i\gamma_\downarrow/2)|e\rangle\langle e| - i\gamma_\uparrow/2|g\rangle\langle g|$ during a time τ before the first induced by the thermal bath jump occurs. We have introduced $\gamma_\downarrow$ (resp. $\gamma_\uparrow$) the rate corresponding to the jump operator $\hat{L}_\downarrow = \sqrt{\gamma_\downarrow}|g\rangle\langle e|$ ($\hat{L}_\uparrow = \sqrt{\gamma_\uparrow}|e\rangle\langle g|$). After time τ, the Qubit state is $|\psi_g^{\rm nj}(\tau)\rangle\frac{\sqrt{p_g^{\rm eq}}}{\sqrt{2}}\left(e^{-i\omega_0\tau-\gamma_\downarrow\tau/2}|e\rangle + e^{-\gamma_\uparrow\tau/2}|g\rangle\right)$. It then undergoes a jump which projects it in the state $\hat{L}_\nu|\psi_g^{\rm nj}(\tau)\rangle$, $\nu = \uparrow,\downarrow$. This first jump determines the value of the effective work $W_{\rm eff}$ provided by the classical source. If $\nu = \uparrow$, then $W_{\rm eff} = 0$ as the Qubit was actually in state $|g\rangle$. The probability of this event is obtained from the norm of the Qubit state just after the first jump, i.e. $p^{(g)}[W_{\rm eff} = 0, \tau] = \langle\psi_g^{\rm nj}(\tau)|\hat{L}_\uparrow^\dagger\hat{L}_\uparrow|\psi_g^{\rm nj}(\tau)\rangle = \gamma_\uparrow e^{-\gamma_\uparrow\tau}p_g^{\rm eq}/2$

which after integrating over all the possible time τ before the first jump occurs gives $p^{(g)}[W_{\rm eff}=0]=p_g^{\rm eq}/2$. Similarly, we find that the probability associated with an effective work $\hbar\omega_0$ (corresponding to jump $\nu=\downarrow$) when starting in state $|g\rangle$ is $p^{(g)}[W_{\rm eff}=\hbar\omega_0]=p_g^{\rm eq}/2$. We can in a similar way look at the evolution when starting with a initial Qubit state $\sqrt{p_e^{\rm eq}}|e\rangle$, with $p_e^{\rm eq}=1-p_g^{\rm eq}$. Once again, the value of the effective work is determines by the first jump: $-\hbar\omega_0$ for a jump $\nu=\uparrow$ and 0 for a jump $\nu=\downarrow$, with probabilities $p^{(e)}[W_{\rm eff}=-\hbar\omega_0]=p^{(e)}[W_{\rm eff}=0]=p_e^{\rm eq}/2$. These results as well as the thermodynamical quantities Q, W, $\Delta E_{\rm res}$, $W_{\rm eff}$ are gathered for that example in the table I. So as to evidence the differences with the classical case, we consider a slightly different situation. Starting to the same initial thermal mixture, we now couples the system to a incoherent classical source which prepares a statistical mixture of states $|e\rangle$ and $|g\rangle$ with equal probability, and let it evolve in contact with the thermal bath at temperature T. We now perform the same analysis as previously. We consider a trajectory starting in $|\psi_i\rangle=\sqrt{p_g^{\rm eq}}|g\rangle$. After interacting with the incoherent source, the Qubit is either in state $\sqrt{p_g^{\rm eq}/2}|g\rangle$ and the source has provided a work $W=0$, either in state $\sqrt{p_g^{\rm eq}/2}|e\rangle$ and the source has provided a work $W=\hbar\omega_0$. It is easy to find that starting with the state $\sqrt{p_e^{\rm eq}}|e\rangle$, the two states after the interaction are $\sqrt{p_e^{\rm eq}/2}|g\rangle$ (corresponding work $W=-\hbar\omega_0$) and $\sqrt{p_e^{\rm eq}/2}|e\rangle$ (W = 0). During the rest of the trajectory, the Qubit is always in an energy eigenstate and no more work is exchanged with the source, so that the effective work for the whole trajectory is reduced to the work provided by the source when it is coupled to the qubit (classical case). As a consequence, we do not have to wait until the first jump induced by the reservoir to know the effective work provided by the source. One then gets: $\langle e^{-W_{\rm eff}[\gamma]}\rangle=\langle e^{-W[\gamma]}\rangle=1$.

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